Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 280 °C

Global applicability domain: Inside

Local applicability domain index: 3.33e-01

Confidence level: 5.30e-01

Nearest Neighbors from the Training Set

Image not found
Carbaryl
Measured: 315
Predicted: 297

Image not found
N-Butylbenzenesulfonamide
Measured: 314
Predicted: 286

Image not found
Ethyl benzylcarbamate
Measured: 230
Predicted: 255

Image not found
Carbamic acid, phenyl-, ethyl ester
Measured: 238
Predicted: 260

Image not found
Ethyl oxanilate
Measured: 280
Predicted: 295